

Quantum discord in quantum computation

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Abstract. Quantum discord is a measure of the quantumness of correlations. After reviewing its different versions and properties, we apply it to the questions of quantum information processing. First we show that changes in discord in the processed unentangled states indicate the need for entanglement in the distributed implementation of quantum gates. On the other hand, it was shown that zero system-environment discord is a necessary and sufficient condition for applicability of the standard completely positive description of the system’s evolution. We demonstrate that this result does not translate into useful quantum process tomography. Depending on the details of the preparation procedure only absence of any initial correlations may guarantee consistency of the process tomography.

1. Introduction

What makes correlations quantum? What makes quantum computer tick? There is no definite answer to these questions, even if entanglement is a primary suspect. It is crucial in performing tasks that cannot be implemented by local operations and classical communications (LOCC), its presence in the system is a natural telltale that something non-local is afoot, and one entangling gate is a part of universal sets of gates [1, 2].

Nevertheless, the story is not so simple. The “sausage” or “four and a half tatami teahouse” states [3] are nine orthogonal pure product states that are shared between the two parties — A(lice) and B(ob). Despite absence of entanglement Alice and Bob cannot distinguish between them by LOCC. Similarly the DQC1 algorithm demonstrates speed up without entanglement [4].

Quantum discord [5, 6] is one of the measures of quantum correlations. We review its three versions and their properties in the next Section. Since its introduction it was found to be related to the efficiency of various Maxwell’s demons [7, 8], quantum phase transitions [9, 10], and quantum state merging [11, 12]. It was also argued that zero discord is a necessary and sufficient condition for the evolution of a system to be of a completely positive type [14, 15], thus being amenable to a relatively simple characterization, in quantum tomography.

We present two of its uses. First, ability to create entanglement is necessary for execution of two-qubit quantum gates even when they are applied to unentangled states and create no entanglement. Changes in discord indicate the failure of a local implementation. Second, having a zero system-environment discord does not guarantee that the resulting tomographic description

is an adequate representation of the relevant gate action. Hence zero discord is not directly related to a “simple” evolution of the system.

2. Three types of discord

2.1. Correlations and entropies

The Shannon entropy [16] of a classical discrete probability distribution over a random variable A with values a , $p(a) \equiv p_a$, is defined by $H(A) = -\sum_a p_a \log p_a$. Entropy of the joint probability distribution over AB , $H(AB)$, is defined analogously. The Bayes theorem relates joint and conditional probabilities,

$$p(a, b) = p(a|b)p(b) = p(b|a)p(a), \quad (1)$$

where $p(a|b)$ is a conditional probability of $A = a$ given that $B = b$. The conditional entropy of A given B ,

$$H(A|B) = \sum_b p_b H(A|b) = -\sum_{a,b} p(a, b) \log p(a|b) \quad (2)$$

is a weighted average of the entropies of A given a particular outcome of B .

Correlations between two probability distributions are measured by the symmetric mutual information. It has two equivalent expressions [16],

$$I(A : B) = H(A) + H(B) - H(A, B) ; J(A : B) = H(A) - H(A|B) = H(B) - H(B|A). \quad (3)$$

Quantum-mechanical (von Neumann) entropy [1, 2, 17] of a system with a density operator ρ is defined as $S(\rho) = -\text{tr } \rho \log \rho$. It minimizes the Shannon entropy of probability distributions that result from rank-1 positive operator-valued measures (POVMs) that are applied to the state ρ . The minimum is reached on a probability distribution A_ρ^Π that results from a projective measurement $\Pi = \{\Pi_a, a = 1, \dots, d\}$, $\sum_a \Pi_a = \mathbb{1}$, $\Pi_a \Pi_b = \delta_{ab} \Pi_a$, which is constructed from the eigenstates of ρ ,

$$S(\rho) = \min_{\Pi} H(A_\rho^\Pi), \quad (4)$$

i. e.,

$$S(\rho) = H(A_\rho^{\Pi^*}), \quad \rho = \sum_a p_a \Pi_a^*, \quad p_a \geq 0, \quad \sum_a p_a = 1. \quad (5)$$

The first expression for mutual information has an obvious quantum generalization,

$$I(\rho_{AB}) := S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \quad (6)$$

and represents the total amount of quantum and classical correlations [18].

To obtain a quantum version of $J(A : B)$, it is necessary to determine a conditional state of the subsystem B [8]. Given a complete projective measurement Π on A , a quantum definition of J follows its interpretation as the information gained about the system B from the measurement on A [5],

$$J^{\Pi^A}(\rho_{AB}) := S(\rho_B) - S(\rho_{B|\Pi^A}), \quad (7)$$

where the conditional entropy is now given by $S(\rho_{B|\Pi^A}) := \sum_a p_a S(\rho_{B|\Pi_a})$.

The post-measurement state of B that corresponds to the outcome $A = a$ is

$$\rho_{B|\Pi_a} = (\Pi_a \otimes \mathbb{1}_B \rho_{AB} \Pi_a \otimes \mathbb{1}_B) / p_a, \quad p_a = \text{tr } \rho_A \Pi_a, \quad (8)$$

while the state of B remains unchanged, $\rho_B = \text{tr}_A \rho_{AB} = \sum_a p_a \rho_{B|\Pi_a}$.

2.2. Discords D_1 and D_2

Unlike their classical counterparts, the quantum expressions are generally inequivalent and $I(\rho_{AB}) \geq J^{\Pi^A}(\rho_{AB})$ [5, 6]. The difference between these two quantities is

$$D_1^{\Pi^A}(\rho_{AB}) := S(\rho_A) + S(\rho_B|\Pi^A) - S(\rho_{AB}). \quad (9)$$

Its dependence on the measurement procedure is removed by minimizing the result over all possible sets of Π , resulting in the quantum discord [5]

$$D_1^A(\rho_{AB}) := \min_{\Pi^A} D_1^{\Pi^A}(\rho_{AB}). \quad (10)$$

Similarly,

$$J_1^A(\rho_{AB}) := \max_{\Pi^A} J^{\Pi^A}(\rho_{AB}). \quad (11)$$

It is possible to define the discord when the difference is minimized over all possible POVM Λ^A [6]. However, unless stated otherwise we restrict ourselves to rank 1 projective measurements.

An explicit form of a post-measurement state will be useful in the following text. We denote this state as $\rho'_X \equiv \rho_X^{\Pi^A}$, where the subscript X stands for A , B , or AB , and use the former expression if it does not lead to confusion. After a projective measurement Π^A , the state of the system becomes

$$\rho'_{AB} = \sum_a p_a \Pi_a \otimes \rho_B^a, \quad (12)$$

where p_a and $\rho_B^a \equiv \rho_{B|\Pi_a}$ are given by Eq. (8).

The discord of the state ρ_{AB} is zero if and only if it is a mixture of products of arbitrary states of B and projectors on A [5],

$$\rho_{AB} = \sum_a p_a \Pi_a \otimes \rho_B^a, \quad p_a \geq 0, \quad \sum_a p_a = 1. \quad (13)$$

By using this decomposition and properties of the entropy of block-diagonal matrices [20] we can identify $J^{\Pi^A}(\rho_{AB}) \equiv I(\rho'_{AB})$, because $S(\rho'_A) = H(A_\rho^\Pi)$ and

$$S(\rho'_{AB}) = H(A_\rho^\Pi) + S(\rho_B|\Pi^A). \quad (14)$$

The discord is not a symmetric quantity: it is possible to have states with $D_1^A(\rho_{AB}) \neq D_1^B(\rho_{AB})$.

Another possibility is to set

$$J_2^{\Pi^A} := S(\rho_A) + S(\rho_B) - [H(A_\rho^\Pi) + S(\rho_B|\Pi^A)] = S(\rho_A) + S(\rho_B) - S(\rho'_{AB}), \quad (15)$$

arriving to the quantum discord as defined in [7]

$$D_2^A(\rho_{AB}) := \min_{\Pi} [H(A_\rho^\Pi) + S(\rho_B|\Pi^A)] - S(\rho_{AB}), \quad (16)$$

where the quantity to be optimized is a sum of post-measurement entropies of A and B . Using Eq. (4) we see that $D_1 \leq D_2$. It is also easy to see that $D_1 = 0 \Leftrightarrow D_2 = 0$. Using Eqs. (12) and (14) we obtain a different expression for D_2 :

$$D_2^{\Pi^A}(\rho_{AB}) = S(\rho_{AB}^{\Pi^A}) - S(\rho_{AB}). \quad (17)$$

Since the definition of the discord(s) involves optimization, the analytic expressions are known only in some particular cases. Moreover, typically it is important to know whether the discord is zero or not, while the numerical value itself is less significant.

2.3. Zero discord and D_3

It follows from Eq. (13) that if the spectrum of a reduced state $\rho_A = \sum_a p_a \Pi_a$ is non-degenerate, then its eigenbasis gives a unique family of projectors Π that results in the zero discord for ρ_{AB} . Hence, a recipe for testing states for zero discord and for finding the optimal basis is to trace out a subsystem that is left alone (B), to diagonalize ρ_A and to calculate the discord in the resulting eigenbasis.

If the state ρ_A is degenerate, a full diagonalization should be used. For the state with the form of Eq. (13), each of the reduced states ρ_B^a can be diagonalized as

$$\rho_B^a = \sum_b r_b^a P_a^b, \quad P_a^b P_a^{b'} = \delta^{bb'} P_a^b. \quad (18)$$

The eigendecomposition of the state ρ_{AB} then easily follows. Writing it as

$$\rho_{AB} = \sum_{a,b} w_a r_b^a \Pi_a \otimes P_a^b, \quad (19)$$

it is immediate to see that its eigenprojectors are given by $\Pi_a \otimes P_a^b$. Hence, if ρ_B has a degenerate spectrum, but ρ_{AB} does not, the structure of its eigenvectors reveals if it is of a zero or nonzero discord. Hence we established [8]

Property 1. The eigenvectors of a zero discord state $D_1^A(\rho_{AB}) = 0$ satisfy

$$\rho_{AB}|ab\rangle = r_{ab}|ab\rangle, \quad \Rightarrow \quad |ab\rangle\langle ab| = \Pi_a \otimes P_a^b. \quad (20)$$

□

This consideration leads to the simplest necessary condition for zero discord [19]:

Property 2. If $D_1^A(\rho_{AB}) = 0$, then $[\rho_A \otimes \mathbb{1}_B, \rho_{AB}] = 0$. Hence a non-zero commutator implies $D_1^A(\rho_{AB}) > 0$. □

Naturally, if the state has zero discord, and the eigenbasis is only partially degenerated, we can use it to reduce the optimization space. On the other hand, the diagonalizing basis Π_* is not necessarily the optimal basis $\hat{\Pi}$ or $\check{\Pi}$ that enters the definition of D_1 or D_2 , respectively. Consider, for example, a two-qubit state

$$\rho_{AB} = \frac{1}{4}(\mathbb{1}_{AB} + b\sigma_A^z \otimes \mathbb{1}_B + c\sigma_A^x \otimes \sigma_B^x), \quad (21)$$

where σ_X^a are Pauli matrices on the relevant spaces, $X = A, B$, and the constants b and c are restricted only by the requirements that ρ_{AB} is a valid density matrix. For this state $\rho_B = \mathbb{1}/2$ and $\rho_A = \text{diag}(1+b, 1-b)/2$. After the measurement in the diagonalizing basis $\Pi^z = ((\mathbb{1} + \sigma^z)/2, (\mathbb{1} - \sigma^z)/2)$ the conditional state of B becomes

$$\rho_{B|\Pi_\pm^z} = \mathbb{1}/2, \quad (22)$$

and the conditional entropy is maximal, $S(\rho_{B|\Pi^z}) = \log 2$.

On the other hand, in the basis $\Pi^x = ((\mathbb{1} + \sigma^x)/2, (\mathbb{1} - \sigma^x)/2)$ the probabilities of the outcomes are equal, $p_+ = p_- = 1/2$, but the post-measurement states of B are different from the maximally mixed one,

$$\rho_{B|\Pi_\pm^x} = \frac{1}{2}(\mathbb{1} \pm c\sigma^x), \quad (23)$$

so the entropy $S(\rho_{B|\Pi^z}) \geq S(\rho_{B|\Pi^x})$.

This discrepancy motivates us to define a new version of the discord [8]:

$$D_3^A(\rho_{AB}) := S(\rho_A) - S(\rho_{AB}) + S(\rho_{B|\Pi_*^A}), \quad (24)$$

where Π_*^A is the set of eigenprojectors of ρ_A . For the degenerate case it can be introduced using the continuity of entropy in finite-dimensional systems [20]. By applying Eq. (4) to the subsystem A we find that D_3 simultaneously holds the analog of Eq. (2.2),

$$J_3(\rho_{AB}) \equiv I(\rho_{AB}^{\Pi_*^A}), \quad (25)$$

and of Eq. (17),

$$D_3(\rho_{AB}) \equiv S(\rho_{AB}^{\Pi_*^A}) - S(\rho_{AB}). \quad (26)$$

We also arrive to the following ordering of the discord measures:

$$D_1^A \leq D_2^A \leq D_3^A. \quad (27)$$

There are several important cases when the measures of discord coincide. Most importantly, they vanish simultaneously:

Property 3. $D_1 = 0 \Leftrightarrow D_2 = 0 \Leftrightarrow D_3 = 0$.

The proof follows from Eqs.(13) and (27). \square .

For pure states the discord is equal to the degree of entanglement,

$$D_i^A(\phi_{AB}) = S(\phi_A) = E(\phi_{AB}), \quad i = 1, 2, 3. \quad (28)$$

Discord is also independent of the basis of measurement if the state is invariant under local rotations [5]. Finally, if A is in a maximally mixed state, then $D_1^A = D_2^A$.

These coincidences make it interesting to check when the discords D_1 and D_2 are different. By returning to the measurement-dependent versions of the discords, we see that

$$D_1^{\Pi^A}(\rho_{AB}) = D_2^{\Pi^A}(\rho_{AB}) - [H(A_\rho^{\Pi}) - S(\rho_A)]. \quad (29)$$

Assume that $D_2^{\Pi^A}(\rho_{AB})$ reaches the minimum on the set of projectors $\tilde{\Pi}$, which are not the eigenprojectors of ρ_A . In this case $H(A_\rho^{\tilde{\Pi}}) - S(\rho_A) > 0$, so we can conclude that the strict inequality $D_1^A < D_2^A$ holds, because

$$\begin{aligned} D_1^A(\rho_{AB}) &\leq D_1^{\tilde{\Pi}}(\rho_{AB}) \\ &= D_2^A(\rho_{AB}) - [H(A_\rho^{\tilde{\Pi}}) - S(\rho_A)] < D_2^A(\rho_{AB}). \end{aligned} \quad (30)$$

For example, the state of Eq. (21), with $b = c = \frac{1}{2}$, satisfies $D_1^A \approx 0.05$, $D_2^A \approx 0.20$ and $D_3^A \approx 0.21$.

2.4. Some applications

The discord $D_1^A(\rho)$ has an operational meaning through quantum state merging [11, 12]. Different restrictions on the local Maxwell demons that operate on the subsystems, as compared to the power of a global demon, lead to the differences in maximal work extraction that are determined by the discords D_2^A and D_3^A [7, 8]. Further work on the discord in quantum open systems can be found in [13].

Since zero discord is thought to represent absence of quantum correlations, it is interesting to investigate the following question. Consider a set of pure orthogonal bipartite states, each of which may have a different prior probability, with the ensemble density matrix ρ_{AB} . Does the value of $D(\rho_{AB})$ tell us something about the ability to perfectly distinguish these states by local operations and classical communication (LOCC)? The answer is negative [8]: there is no relation between $D(\rho_{AB})$ and local distinguishability, as illustrated in Table 1. We use the nine teahouse states

$$|1\rangle \otimes |1\rangle, \quad |0\rangle \otimes |0 \pm 1\rangle / \sqrt{2}, \quad |2\rangle \otimes |1 \pm 2\rangle / \sqrt{2}, \quad |1 \pm 2\rangle \otimes |0\rangle / \sqrt{2}, \quad |0 \pm 1\rangle |2\rangle / \sqrt{2}, \quad (31)$$

of [3], and the result [21] that any two orthogonal (entangled or not) states can be perfectly distinguished by LOCC to compile the table.

Table 1. Local measurability vs. discord

States	Discord	Locally Distiguishable
9 teahouse states, equal weights	$D^A = D^B = 0$	no
2 product bi-orthogonal states	$D^A = D^B = 0$	yes
2 entangled orthogonal states	$D_1^A > 0$	yes
9 teahouse states, unequal weights	$D_1^A > 0$	no

3. Restricted quantum gates

It is usually thought that quantum computers are potentially faster than their classical counterparts because of the ability to create and use entanglement during the computation [22]. Nevertheless, recent results indicate that it is discord rather than entanglement which is responsible for the speed-up [4, 23, 24, 25].

Using a simple example we show how changes in discord indicate the need for entanglement as a resource even if the processed states are unentangled. More general results may be found in [23]. The non-classicality of quantum gates can be examined by the amount of quantum resources required for the operation of the gate. Our method is to analyze the resources that are needed for a bi-local implementation of a gate.

A CNOT gate can be implemented bi-locally by Alice and Bob if they share one ebit of entanglement per gate use [26]. If they can perform only LOCC they cannot implement this gate even on a restricted set of unentagled inputs that are transformed into unentagled outputs. One such set \mathcal{L} is in Table 2.

Table 2. Four inputs/outputs for the CNOT gate

#	State	#	State
a	$ 1\rangle Y_+\rangle \rightarrow i 1\rangle Y_-\rangle$	c	$ Y_+\rangle X_-\rangle \rightarrow Y_-\rangle X_-\rangle$
b	$ 0\rangle Y_+\rangle \rightarrow 0\rangle Y_+\rangle$	d	$ Y_+\rangle X_+\rangle \rightarrow Y_+\rangle X_+\rangle$

Here $\sigma_y|Y_\pm\rangle = \pm|Y_\pm\rangle$, $\sigma_x|X_\pm\rangle = \pm|X_\pm\rangle$, where $\sigma_{x,y,z}$ are Pauli matrices.

We show that the ability to implement the CNOT gate on \mathcal{L} without shared entanglement allows one to unambiguously discriminate between these non-orthogonal states using just one input copy, which is impossible [17]. Without specifying the local operations of Alice and Bob we classify them according to their action on the state $|Y_+\rangle$. An operation Φ is *flipping* (F) if up to a phase $\Phi(|Y_+\rangle) = |Y_-\rangle$, *non-flipping* (N) if $\Phi(|Y_+\rangle) = |Y_+\rangle$, and undetermined otherwise.

Knowing the type of the operation allows Alice and Bob to narrow down the list of the possible inputs: e.g., Bob's F is incompatible with having input b , while for Alice's operation not to have a definite type excludes both c and d . If one of the operations done is neither F nor N, then the type of other operations allows to determine the input uniquely.

Any pair of outputs can be reset to the original inputs by local unitaries and resent through the gate. For example, if the overall operation was of FF type, the operation $\sigma_z^A \otimes \sigma_x^B$ transforms the outputs $\psi'_a = |1\rangle|Y_-\rangle$ and $\psi'_c = |Y_-\rangle|X_-\rangle$ into the inputs ψ_a and ψ_c .

The operations that implement the gate this time may be of the same type as before, or different. If the gate is such that there is a finite probability of having a different operation type, it will be realized after a finite number of trials. This other type (FN or NF in the above example) will uniquely specify the inputs. If the gate's design is such that a particular pair of inputs is always processed by the same type of operations, then the gate can be used to unambiguously distinguish between one state from this pair and at least one of the two remaining states in a single trial. \square

The operation in the example changes the discord of the ensemble and has been extended in [23] to a more general setting involving a symmetrised type of discord defined as

$$D_2(\rho) := \min[D_2^A(\rho), D_2^B(\rho)] \neq 0. \quad (32)$$

It is however not yet clear if discord is indeed the best measure for this kind of non locality. It is noteworthy to mention that the algorithm described in [4] changes the discord of only one of the parties so that D_2 remains zero throughout the computation.

4. (Non) completely positive maps and discord

4.1. Completely positive maps and gate tomography

Environmental interactions are the major obstacle for practical quantum information processing. Together with the imperfect tailoring of gate Hamiltonians they are responsible for discrepancies between the ideal unitary gates and their experimental realizations. This is why characterization of quantum processes is an essential step in implementing quantum technology. The exposition below is based on [28]. Experimental realization of this discussion is currently in progress.

Usually the transformation of input to output states of an open system is described by completely positive (CP) maps. Any such map $\mathcal{E}(\rho)$ can be seen as a reduction of a unitary evolution of some initially uncorrelated system–environment state $\rho_{AB} = \rho_A \otimes \omega_B$, where the initial states of the system and the environment were ρ_A and ω_B , respectively. Under the joint evolution U_{AB} the state of the system is transformed to

$$\rho'_A \equiv \mathcal{E}(\rho_A) = \text{tr}_B U \rho_{AB} U^\dagger = \sum_a M_a \rho_A M_a^\dagger, \quad (33)$$

where M_a are the Kraus representation matrices [1, 2]. Using the spectral decomposition $\omega = \sum_\nu p_\nu |\nu\rangle\langle\nu|$ one recovers the Kraus matrices from

$$\rho' = \sum_{\mu, \nu} \langle \mu | \sqrt{p_\nu} U | \nu \rangle \rho \langle \nu | \sqrt{p_\nu} U^\dagger | \mu \rangle. \quad (34)$$

This result is based on the absence of prior correlations between the system and the environment.

The action of a given gate is reconstructed using several methods of quantum process tomography. We focus on the standard process tomography, which consists in following. A set of input states $\{\rho_j\}$ is prepared and sent through the process \mathcal{E} . From the knowledge of the input and the reconstructed outputs $\mathcal{E}(\rho_k)$ states the process matrix χ [1, 27, 29] is reconstructed. If K_m , $m = 1, \dots, d^2$ form the basis for operators acting on \mathcal{H}_A , $d = \dim \mathcal{H}_A$, then

$$\mathcal{E}(\rho) = \sum_{m, n} \chi_{mn} K_m \rho K_n^\dagger. \quad (35)$$

For a CP evolution all the eigenvalues of χ are non-negative, and the Kraus matrices are obtained as its (generalized) eigenvectors.

Various mathematical techniques are used to convert the relative frequencies of different measurement outcomes into the states $\mathcal{E}(\rho_k)$. Positivity of states ρ'_j and complete positivity of the process \mathcal{E} are enforced, and its violations by the raw data are interpreted as a result of noise.

The combined state of a system (A) and its environment (B) can be represented in the Fano form

$$\rho_{AB} = \frac{1}{d_A d_B} \left(\mathbb{1}_{AB} + \sum_i \alpha_i \sigma_i^A \otimes \mathbb{1}_B + \sum_j \beta_j \mathbb{1}_A \otimes \sigma_j^B + \sum_{ij} \gamma_{ij} \sigma_i^A \otimes \sigma_j^B \right). \quad (36)$$

Here the σ_i^X , $i = 1, \dots, d_X^2$ represent generators of $SU(d_X)$, while the real vector $\vec{\alpha}$ (or $\vec{\alpha}$) of size $d_X^2 - 1$ is the generalized Bloch vector of the reduced density operator ρ_X . The correlations between subsystems A and B are characterized by

$$\Gamma_{ij} = (\gamma_{ij} - \alpha_i \beta_j) / d_A d_B. \quad (37)$$

Presence of correlations not only can lead to a non-CP evolution of the system, but blurs its boundary with the environment. Part of the controversy surrounding non-CP maps in literature [27] can be traced to this ambiguity as well as to the impossibility of unrestricted creation of arbitrary input states of the system (that are to form a tomographically complete basis in the standard CP paradigm) ρ_j and their correlations with the environment Γ_j .

This situation has an important bearing on the process tomography and action of quantum processing devices. In the following we show that while zero discord $D_A(\rho_{AB})$ ensures a complete positivity of the resulting evolution [14], it does not necessarily translate into a useful tomographic description of the ensuing evolution.

4.2. Role of preparations

State preparation is a vital aspect of quantum process tomography. When initial correlations are present in the input state, the preparation procedure used has considerable impact on the outcome. We discuss two such schemes: state preparation by a measurement and rotations and state preparation by projective measurements [30].

In the former case (Method 1) a single post-selected state that corresponds to a projection operator $\rho_H = \Pi_H$ is used. Once we have performed the projective measurement the required input states are obtained by applying the appropriate matrix from a set of unitary rotation matrices $\{R_a\}$ such that $R_a \rho_H R_a^\dagger = \rho_a$ where ρ_a is run over the tomographically complete set of input states.

Hence the preparation maps for Method 1 are given by

$$\mathcal{P}_a(\rho_{AB}^{\text{in}}) = \frac{1}{p_H} (R_a \Pi_H^A \otimes \mathbb{1}_B) (\rho_{AB}^{\text{in}}) (\Pi_H^A R_a^\dagger \otimes \mathbb{1}_B) = \rho_a \otimes \omega_H, \quad (38)$$

where $p_H = \text{tr}(\Pi_H^A \rho_A^{\text{in}})$ is the probability of detecting the outcome corresponding H , and R_j brings $|H\rangle\langle H|$ to one of the states $\rho_a \equiv |\psi_a\rangle\langle\psi_a|$. The post-preparation state of the environment is dependent on both the initial state ρ_{AB}^{in} and the measurement operator Π_H .

State preparation using *only* measurements (Method 2) utilizes the set of projectors $\{\Pi_a\}$ where $\Pi_a \equiv \rho_a$. Hence the preparation procedure for projective measurements is given by the collection of maps $\{\mathcal{P}_a\}$ where

$$\mathcal{P}_a(\rho_{AB}^{\text{in}}) = \frac{1}{p_a} (\Pi_a^A \otimes \mathbb{1}_B) \rho_{AB}^{\text{in}} (\Pi_a^A \otimes \mathbb{1}_B) = \rho_a \otimes \omega_a. \quad (39)$$

where $p_a = \text{tr}(\Pi_a^A \rho_A^{\text{in}})$ is the probability of detecting the outcome corresponding to Π_j . In this preparation scheme the state of the environment, ω_j depends on the probe state of the system, ρ_k , hence the process matrix will not necessarily be CP.

Lemma 1: Zero discord of the initial state does not guarantee a CP evolution in a tomographic procedure.

Consider the state

$$\rho_{AB}^{\text{in}} = \frac{1}{2} (|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|), \quad (40)$$

which satisfies even a stronger requirement $D^A(\rho_{AB}^{\text{in}}) = D^B(\rho_{AB}^{\text{in}}) = 0$. If the tomographic procedure is based on preparations by measurements, the resulting process matrix χ has the eigenvalues $(1 \pm \sqrt{3}/2, \pm\sqrt{3}/2)$ and hence the evolution is not CP. \square

Preparation by measurement and rotations is guarantied to lead to a CP evolution. However, we should be concerned that the actual state on which the gate will operate is different from the ones prepared in this procedure, and hence the predictive power of the resulting process matrix χ will be low. Having a zero discord does not alleviate this difficulty, as shown below. We consider different reconstruction of process matrices for a generic fixed overall unitary U_{AB} .

Lemma 2: Reconstructed process matrices $\chi_{\mathcal{P}_a}$ that follow from the spanning set of measurement preparations $\{\mathcal{P}_a^A\}$ that are given by projectors Π_a^A , $a = 1, \dots, d_A^2 - 1$, applied to the same initial system–environment state (ρ_{AB}^{in}) , are equal if and only if this initial state is simply separable, $(\rho_{AB}^{\text{in}}) = (\rho_A^{\text{in}}) \otimes (\omega_B^{\text{in}})$.

The sufficient part is obvious. To prove the necessary condition we recall that Kraus matrices form an eigendecomposition of the process matrix, hence from Eq. (34) it follows that all post-selected environmental states ω_k have to have the same spectrum. Hence up to a local reshuffling after the preparation by measurement Π_a

$$\rho_{AB}^{\text{in}} \mapsto \mathcal{P}_a^A(\rho_{AB}^{\text{in}}) = \Pi_a \otimes \omega_B^0. \quad (41)$$

Using Fano decomposition of Eq. (36) we find that for all a the post-measurement state of B is

$$\omega_B^0 = \text{tr}_A \mathcal{P}_a^A(\rho_{AB}^{\text{in}}) = \frac{1}{d_B} (\mathbb{1}_B + \sum_j \beta_j^{\text{in}} \sigma_j^B) + \frac{1}{p_a} \sum_j \left(\sum_i \Gamma_{ij}^{\text{in}} \text{tr}(\Pi_a \sigma_i^A) \right) \sigma_j^B, \quad (42)$$

hence for any j

$$\sum_i \Gamma_{ij}^{\text{in}} \langle \psi_a | \sigma_i | \psi_a \rangle = 0, \quad (43)$$

for all a in all sets of tomographically complete projectors. As a result, $\Gamma_{ij}^{\text{in}} = 0$ so the initial state ρ_{AB}^{in} is indeed a direct product $\rho_A^{\text{in}} \otimes \omega_B^0$. \square

4.3. Examples

We illustrate the differences between the outcomes of Methods 1 and 2 by considering qubits as the system and environment and a CNOT gate with system A as the target being the overall unitary. Let the initial state of joint system AB to be the maximally entangled state $\rho_{\Phi^+} = |\Phi^+\rangle\langle\Phi^+|$ where $|\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$.

The reconstructed process matrices are

$$\chi_1 = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \quad \chi_2 = \frac{1}{2} \begin{pmatrix} 2 & 0 & -1-i & 1 \\ 0 & 0 & 1 & 1+i \\ -1+i & 1 & 2 & 0 \\ 1 & 1-i & 0 & 0 \end{pmatrix}, \quad (44)$$

for Methods 1 and 2, respectively. As follows from Eq. (38), in the former case we have a CP evolution (actually it is an identity $\mathcal{E}_1 = \mathcal{I}$), while χ_2 on the other hand has eigenvalues $(1 + \frac{\sqrt{3}}{2}, -\frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2}, 1 - \frac{\sqrt{3}}{2})$ and hence the reconstructed process is not completely positive. To see why this happens consider the state of the environment after each preparation procedure. We have that all states are different,

$$\omega_H = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \omega_V = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \omega_D = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \omega_R = \frac{1}{2} \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}. \quad (45)$$

While we used a maximally entangled input state, this result holds even for separable inputs. For example, for the input state $\rho_{AB}^{\text{in}} = \frac{1}{2}(\rho_H \otimes \rho_A + \rho_D \otimes \rho_V)$, the process matrix χ_2 has the eigenvalues $\{1.642, 0.507, -0.253, 0.105\}$, so the evolution is still non-CP.

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